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Quantum-chemical calculations of the structure and vibration spectrum of methyl nitrate

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Abstract

© Published under licence by IOP Publishing Ltd. Methyl nitrate vibration spectra theoretical analysis data within the B3LYP density functional theory method in the 6 -31G (d) basis are represented. When optimizing the geometry of the molecule it was found out that methyl nitrate is characterized by one stable conformation: trans-form. Frequency, intensity and forms of normal vibrations are calculated, their comparative analysis with well-known from the literature experimental data is given.

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